

# A hybrid life cycle assessment of water treatment chemicals: an Australian experience

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## Abstract

**Purpose** Life cycle assessment (LCA) of chemicals is usually developed using a process-based approach. In this paper, we develop a tiered hybrid LCA of water treatment chemicals combining the specificity of process data with the holistic nature of input–output analysis (IOA). We compare these results with process and input–output models for the most commonly used chemicals in the Australian water industry to identify the direct and indirect environmental impacts associated with the manufacturing of these materials.

**Methods** We have improved a previous Australian hybrid LCA model by updating the environmental indicators and expanding the number of included industry sectors of the economy. We also present an alternative way to estimate the expenditure vectors to the service sectors of the economy

when financial data are not available. Process-based, input–output and hybrid results were calculated for caustic soda, sodium hypochlorite, ferric chloride, aluminium sulphate, fluorosilicic acid, calcium oxide and chlorine gas. The functional unit is the same for each chemical: the production of 1 tonne in the year 2008.

**Results and discussion** We have provided results for seven impact categories: global warming potential; primary energy; water use; marine, freshwater and terrestrial ecotoxicity potentials and human toxicity potential. Results are compared with previous IOA and hybrid studies. A sensitivity analysis of the results to assumed wholesale prices is included. We also present insights regarding how hybrid modelling helps to overcome the limitations of using IO- or process-based modelling individually.

**Conclusions and recommendations** The advantages of using hybrid modelling have been demonstrated for water treatment chemicals by expanding the boundaries of process-based modelling and also by reducing the sensitivity of IOA to fluctuations in prices of raw materials used for the production of these industrial commodities. The development of robust hybrid life cycle inventory databases is paramount if hybrid modelling is to become a standard practice in attributional LCA.

**Keywords** EIO-LCA · Hybrid LCA · Price sensitivity · Process LCA · Water treatment chemicals

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## 1 Introduction

Chemicals are widely used around the world with global production worth around four trillion US dollars (USD) in

2010 (OECD 2011). In Australia, the chemical industry had a turnover close to 33.6 billion Australian dollars (AUD) in 2010, representing around 10 % of total national manufacturing activity. This sector of the economy also provides materials to other sectors such as food, mining, building and infrastructure, defence, water and wastewater services (PACIA 2011). Such a high level of interconnectedness means that the chemical sector represents an important link in assessing environmental impacts of the supply chain for many industries.

In the water industry, chemicals are used in conventional and membrane processes alike, including coagulation/flocculation, disinfection, filtration and remineralisation. Their contribution to the environmental impacts of water supply has been estimated in previous life cycle assessment (LCA) studies (Friedrich 2002; Mohapatra et al. 2002; Raluy et al. 2005; Barrios et al. 2008; Vince et al. 2008; Lundie et al. 2004), but most of the LCI data for chemicals used in these studies have been developed using a process-based approach (Finnveden et al. 2009; Hischier et al. 2005). Previous research has shown the need to move away from process-based LCA as databases fail to include the breadth and depth of other sectors of the economy (e.g. services) (Majeau-Bettez et al. 2011). A previous study of the basic chemicals sector in Australia has shown that in order to cover at least 87 % of the GHG emissions in this industry sector, it is necessary to include at least 20 different supply chain items from sectors which might normally be overlooked by conventional process modelling (e.g. meat products) (Lenzen and Murray 2009).

Environmentally extended input–output (EEIO) data have been recognised as a valid approach to remove this truncation error issue because it enables the inclusion of all interactions between the economy and the entity under assessment. EEIO data for chemicals have been used to fill data gaps in past LCA studies (Racoviceanu et al. 2007; Stokes and Horvath 2010), in particular in the USA, using tools such as the Economic Input–Output Life Cycle Assessment (EIO-LCA) (Carnegie Mellon University Green Design Institute 2012). However, one limitation of using IO data is the averaging of data associated with different chemicals within the various industry sub-sectors. Hybrid modelling has been developed to overcome the issues of completeness and averaging by combining the holistic nature of EEIO data with the specificity of process-based modelling (Suh 2003; Suh and Huppes 2005).

Hybridisation of life cycle inventory (LCI) databases has been discussed in recent years at the global level (Weidema 2011) and in the USA (Suh and Lippiatt 2012) using an integrated hybrid approach (Suh and Huppes 2005). It is expected that hybrid databases will enable better and faster LCI modelling by enabling combined analysis of the interactions of the economy at the macro level with the system under study at the process level. In the case of water treatment chemicals, such a database should ideally consider

the possible impacts on the final LCA results from fluctuations in the prices of raw materials used to manufacture these industrial commodities (WRF 2009).

The objective of this paper is to present hybrid LCA results of water treatment chemicals and compare them with the results of previous Australian hybrid and IO models. Additional insights are given about updating environmental data for different input–output industry groups (IOIGs), estimating expenditures to the service sectors of the economy and the sensitivity of the results to the assumed wholesale prices.

## 2 Methods

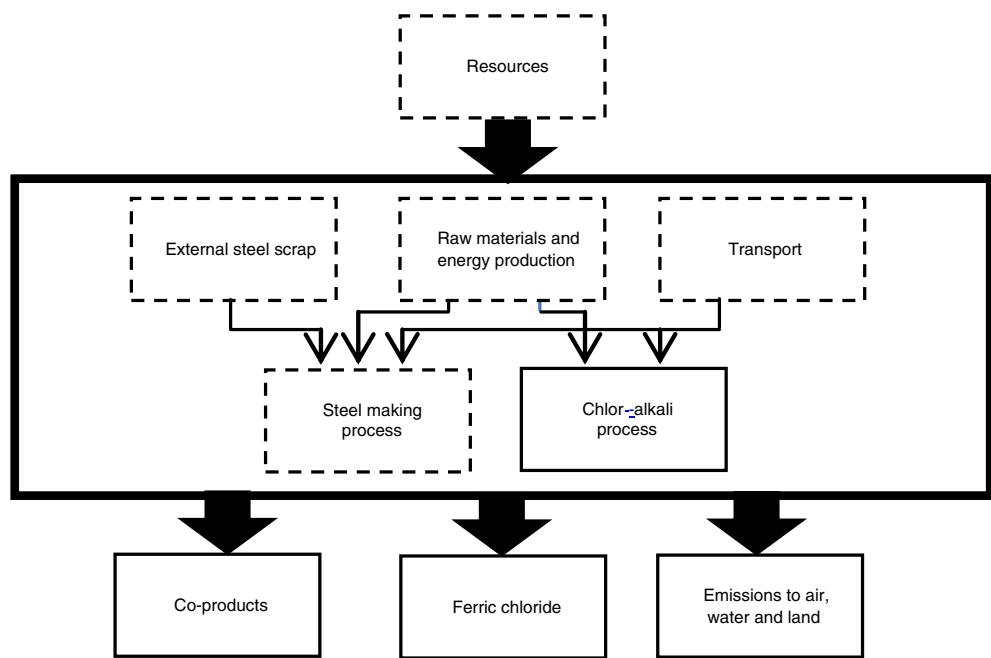
Hybrid LCA aims to quantify in one single model the environmental impacts of a product or service by combining the completeness of a top-down technique and IO-based LCA and the specificity of bottom-up process-based LCA (Suh and Huppes 2005). We include in this study a detailed description of tiered hybrid model construction which has been divided into three components to make it more manageable. The functional unit for each chemical is the production of 1 tonne of product in the year 2008, with all chemicals manufactured by the IOIG 1803 named “Basic chemical manufacturing” except calcium oxide which is produced by the IOIG 2003 “Cement, lime and ready-mixed concrete”.

### 2.1 Process modelling

To create new data relevant to a broad range of stakeholders, the chemicals for assessment in this research project were prioritised using a 3-year rolling survey completed by six Australian water utilities which together serve 66 % of the national population (Alvarez-Gaitan et al. 2011). Based on total annual mass consumed by the water sector, the chemicals of highest priority were sodium hydroxide (50 % w/w), sodium hypochlorite (13 % w/w), ferric chloride (42 % w/w), aluminium sulphate (47 % w/w), fluorosilicic acid (22 % w/w), calcium oxide and chlorine gas.

After having obtained initial consumption information from water utilities, we then engaged with different chemical producers around Australia to gather on-site data about their production processes. This process analysis included questionnaires, interviews and visits to their facilities. Following initial engagement and exploratory data gathering, two plants for chlor-alkali chemicals (ferric chloride, chlorine gas, caustic soda and sodium hypochlorite) were assessed and one plant each for the remaining chemicals (calcium oxide, fluorosilicic acid and aluminium sulphate). Process data were allocated on a mass basis where required. For illustrative purposes, Fig. 1 provides details of the processes included in the process modelling of ferric chloride.

**Fig. 1** System boundaries for process-based modelling of ferric chloride production (broken lines represent the use of the GaBi 5 database (PE International 2012) and the continuous lines represent the data gathered by the authors)



## 2.2 Pure IO model

Leontief pioneered the use of input–output analysis (IOA) to analyse environmental issues (Leontief 1970). For LCA purposes, the total environmental impact of a particular system under analysis is the result of adding the burdens at zero (direct) and higher (indirect) orders (see [Electronic Supplementary Material C](#) for additional details). The burden at zero order is calculated by multiplying the revenues per unit of the system under study (e.g. AUD/tonne) by the environmental interventions matrix which is expressed in impact units per AUD (e.g. kilograms CO<sub>2</sub> equivalent/AUD). The environmental intervention matrix is calculated by dividing the resource usage (e.g. primary energy) or emissions data (e.g. emissions to air) per industry sector by the respective financial output of each industry sector of the economy (see [Electronic Supplementary Material A](#) for additional details). These figures are commonly published by statistical bureaux or government agencies around the world. In Australia, the financial output per industry sector was taken from the latest IO tables published by the Australian Bureau of Statistics (ABS) ([2011b](#)), primary energy and water use data were sourced from national energy and water accounts (ABS [2011a, 2012](#)), data regarding GHG emissions were sourced from the Australian Greenhouse Emissions Information System (AGEIS) (AGEIS [2012](#)) and data on toxic emissions to water, air and soil were sourced from the National Pollution Inventory (DSEWPC [2011](#)). The most recent release of input–output tables from the ABS is associated with 2008 and we have used it as the reference year for all our data sources.

These data sources required some adjustments before integration with the IO tables. While the input–output

framework in Australia is built upon 111 IOIGs, toxic emissions, primary energy, water and GHG data are organised according to the latest Australian and New Zealand Standard Industry Classification scheme released in 2006, which includes 19 divisions, 86 subdivisions, 214 groups and 506 classes, with figures publicly available mainly at the division and subdivision level. Toxic emissions, primary energy, water and GHG data were, therefore, allocated to the IOIGs using a mapping table (see [Electronic Supplementary Material A](#) for additional details). When data were only available at the division level, disaggregated physical data (Foran et al. [2005](#)) were used to calculate the relative contribution of each class within each division and then allocated to the IOIGs accordingly. For example, GHG data about division B “Mining” (60,022.93 Gg) are given with details of only two out of the six subdivisions. By mapping these data, we then have figures for the IOIG 0601 “Coal mining” (31,812.43 Gg) and IOIG 0701 “Oil and gas extraction” (18,016.39 Gg) but a single figure (10,193.21 Gg) for the remaining IOIGs, which are 0801 “Iron ore mining”, 0802 “Non-ferrous metal ore mining”, 0901 “Non-metallic mineral mining” and 1001 “Exploration and mining support services”. By using previous physical data at the class level, we have been able to allocate 14.51 % of this figure to IOIG 0801 Iron ore mining, 51.63 % to IOIG 0802 Non-ferrous metal ore mining, 30.84 % to 0901 Non-metallic mineral mining and 3.02 % to IOIG 1001 Exploration and mining support services.

Toxic emissions data also required further adjustments to enable characterisation. Emissions to water were allocated to seawater or freshwater based on the postcode of the emitting facility. Emissions to soil were allocated to agricultural soil if the sector belongs to the agriculture, forestry and fishing

division or industrial soil if not. Emissions to air did not require further allocation.

The burden at higher orders includes the interactions of the entity under study with the rest of the economy and these were calculated by multiplying the environmental matrix by the Leontief inverse and the expenditure vector of the entity under study (see [Electronic Supplementary Material C](#) for additional details). The Leontief inverse is calculated by applying matrix inversion to the result of subtracting the transaction matrix from the identity matrix (see [Electronic Supplementary Material B](#) for additional details). The transaction matrix is commonly published by statistical agencies and describes the monetary flows from industry  $i$  to industry  $j$  in the economy. In Australia, this matrix is taken from the following IO table provided by the ABS, “Table 9, direct requirement coefficients, indirect allocation of imports” (ABS 2011b). By using this table, we assume that imported products are added to the domestic supply of goods in their respective industry sector and then this supply is ascribed to the different industry sectors which use them.

The expenditure vector is calculated by allocating the expenditures of the entity under study to different sectors of the economy. However, this allocation requires two modifications: firstly, the transformation of expenditures from a commodity basis to an industry basis and, secondly, the conversion from purchasers’ prices to basic prices. The first modification requires the use of the supply coefficient matrix which is calculated by dividing the cells in each row of “Table 1, Australian supply table, supply by product group by industry” (ABS 2011b) by the total output of each product group per row, which gives us the proportion of total commodity output being produced by each industry. The second modification uses a ratio of purchasers’ prices to basic prices which is calculated from “Table 4, reconciliation of flows at basic prices and at purchasers’ prices by product group” (ABS 2011b) (see [Electronic Supplementary Material A](#) for additional details).

Expenditure vectors are, in principle, easier to gather than process data as many enterprise resource planning systems (e.g. SAP software) can give access to a large amount of financial information in a matter of seconds. However, these figures are often unavailable due to confidentiality restrictions, as was the case during this study. Consequently, these financial flows were estimated using process-based LCI data and market prices from different sources (USGS 2011). This approach is valid for most of the variable costs (e.g. raw materials) which were gathered in the previous process-based life cycle inventory stage and represent the majority of expenditures in manufacturing/mining/agricultural facilities. In the case of fixed costs (e.g. services), however, process data are inadequate for estimating expenditures to other sectors of the economy. To overcome this, we estimated the value of services required by using a ratio of variable costs to fixed costs and the

average proportion of commodity usage per industry sector. For example, in the case of chlor-alkali plants, the relationship between variable costs and fixed costs is 80:20 (EIPPCB 2011); combining this information with the average profile of commodity usage in the basic chemical industry (ABS 2011b), it is possible to estimate the expenditure to service sectors of the economy (see [Electronic Supplementary Material A](#) for additional details).

### 2.3 Building a tiered hybrid model

Hybridising process and IO models require further consideration of two issues: the location of the interface and the potential for double counting. The first one requires an understanding of the supply chain and that no major process is being modelled using IO data. The key concept to understand here is “depth”, which means the order in which each industry sector is included in the process model in GaBi 5 (PE International 2012), being zero order the IOIG to which the site under analysis belongs. For example, the chlor-alkali facility belongs to the IOIG 1803 “Basic chemicals” (zero order) and the electricity used in this facility is supplied by the IOIG 2605 “Electricity transmission, distribution, on selling and electricity market operation” (first order), which at the same time is being supplied by the IOIG 2601 “Electricity generation” (second order). The black coal used in the power station is been hauled by the IOIG 4601 “Rail transport” (third order) and mined by the IOIG 0601 Coal mining (fourth order). In GaBi 5 (PE International 2012), the detailed data associated with the supply of electricity in New South Wales include the mining of black coal, the transport to the power station and the production and transmission of electricity (including losses). As a result, in the case of electricity being used at the chlor-alkali facility, we have located the interface between the process and IO model at the fourth order (or layer) of the supply chain. A similar procedure should be undertaken for each input required in the production of the other chlor-alkali chemicals, aluminium sulphate, calcium oxide and fluorosilicic acid. Additional details of this are given in the [Electronic Supplementary Material C](#).

The second issue deals with potential double counting. Input–output-based LCA has better coverage than process-based LCA but there is a risk of counting the impacts twice when using hybrid LCA. Various solutions to this issue have been proposed (Rowley et al. 2009; Lenzen and Crawford 2009; Suh and Huppes 2005). In this study, we calculated system incompleteness factors for the higher orders of each industry sector of the economy and applied these to the expenditure vector of each chemical in the IO analysis according to the depth of the process-based LCI (Rowley et al. 2009). This results in a process-based model representing the lower orders of the system, while the higher orders are represented as a fraction of the total IO results. Those sectors

not included in the process-based model and relevant to the operation of the entity under analysis (e.g. services) are fully represented by the IO model. Additional details of this are given in the [Electronic Supplementary Material C](#).

#### 2.4 Life cycle impact assessment

Global warming potentials used in the AGEIS and, therefore, applied here are the 100-year global warming potentials (GWP<sub>s</sub>) published in the 1995 IPCC Second Assessment Report (IPCC 1995). Water use in the IO modelling is defined as “water consumption” in accordance with the definition used by the ABS (2012), and due to the primarily urban/industrial use of water in the chemical industry, it is considered as an elementary flow and is not further characterised. As global consensus on water use characterisation proceeds (Kounina et al. 2013), it may be interesting to develop this aspect further. Australian characterisation factors for ecotoxicity and human toxicity potential using dichlorobenzene (DCB) equivalents (Lundie et al. 2001) are used to guarantee compatibility between the outputs of process-based and IO modelling (see details in the [Electronic Supplementary Material A](#)). Primary energy does not require further characterisation.

### 3 Results and discussion

Process-based, input–output and hybrid results are presented for the chosen chemicals in Table 1 for the following impact categories: GWP, primary energy use (PE), water use (WU), freshwater aquatic ecotoxicity potential (FETP), marine aquatic ecotoxicity potential (METP), terrestrial ecotoxicity potential (TETP) and human toxicity potential (HTP).

#### 3.1 Environmental indicators

For global warming potential, IOA was able to estimate values for the chlor-alkali chemicals (sodium hydroxide, sodium hypochlorite, ferric chloride and chlorine gas) as 82–135 % of the process-based figure (see Table 1). The scale of the IOA results compared to the process-based results for the other chemicals was 262 % for aluminium sulphate, 809 % for fluorosilicic acid and 42 % for calcium oxide (see Table 1). Overall, these results indicate that IOA was better at estimating the GWP of chlor-alkali chemicals than it did for the remaining chemicals. For aluminium sulphate and fluorosilicic acid, the price volatility of some raw materials (e.g. phosphate rock and sulphuric acid) might have a significant impact on the final results of IOA which are further discussed in Section 3.3. The apparent underestimation of GWP by the IOA of calcium oxide (i.e. lime) is particularly notable. Analysing this result, we identified (see figures in Table 1) that the zero-order contribution

is smaller (159 kg CO<sub>2</sub>-eq) than the higher orders (387 kg CO<sub>2</sub>-eq), which does not acknowledge that most of the emissions from lime production are associated with the decarbonisation of limestone and the combustion of fossil fuels in the kiln which are located at the zero order of the IO model. This can be explained by the relatively high contribution to the financial output of this IOIG by ready-mixed concrete (approximately 70 % of the IOIG), which has a much smaller zero-order GWP. The emissions for lime/cement production are, therefore, artificially lowered by the inclusion of ready-mixed concrete in the IOIG.

For primary energy, results using IOA were 52–101 % of the process-based figures for the chlor-alkali chemicals, 102 % for aluminium sulphate, 164 % for fluorosilicic acid and 24 % for calcium oxide (see Table 1). For the “Basic chemical” sector, including only the first layer of suppliers would result in a system completeness of only 42.8 % which is associated with the use of natural gas for fuel, power and as a feedstock in the production of chemicals such as ammonia, methanol and ethylene. However, in the particular case of water treatment chemicals in this study, little primary energy is being supplied with the exception of natural gas used in steam production for sodium hydroxide evaporation. For calcium oxide, which belongs to the IOIG Cement, lime and ready-mixed concrete product manufacturing, the system completeness factor at the first order is 36.8 % although natural gas is used in the kiln. These over and under estimations at the first order are compensated by hybrid modelling, giving us a more meaningful result by disaggregating both industry sectors using process-based LCI data at lower orders while maintaining the comprehensiveness of the system boundary via IO modelling.

Water use at the first order for the Basic chemicals sector accounts for 21.8 % of the total water use result obtained using IO modelling. This means the majority of water is being used upstream in the chemical supply chain; however, for all the chemicals in this study, the process-based results are consistently higher than the IO results. Although water use data have a better resolution per industry sector than GHG emissions or primary energy use data, we consider that the price paid in industry sectors connected to higher levels in the supply chain is probably substantially lower than that paid at the (urban) chemical manufacturers’ site. Additionally, the relationship between energy production and water use for chlor-alkali chemicals is particularly relevant. These chemicals use a substantial amount of electricity in their production processes (e.g. electrolysis), and as a result, we might expect the IOA model to identify a substantial use of water at higher order levels associated with electricity generation. However, water is “used” but not “consumed” in many power stations in the Australian states of New South Wales and Victoria as they use once-through cooling systems and this “usage” is not registered as a regular expenditure in the power

**Table 1** Process-based, input–output and hybrid LCA results for selected water treatment chemicals

Chemical	Impact category	Process LCA	Input–output LCA			Hybrid LCA
			Zero order	Higher order	Total	
Caustic soda (50 % w/w)	GWP, kg CO <sub>2</sub> -eq	7.91E+02	2.74E+02	7.96E+02	1.07E+03	1.01E+03
	PE, GJ	9.36E+00	3.03E+00	5.19E+00	8.23E+00	9.65E+00
	WU, ML	1.03E−01	9.75E−04	1.11E−03	2.08E−03	1.03E−01
	FETP, kg DCB-eq	2.93E−01	7.37E−03	1.09E−02	1.83E−02	2.97E−01
	METP, kg DCB-eq	2.17E+04	5.24E+02	6.75E+02	1.20E+03	2.19E+04
	TEP, kg DCB-eq	1.16E+01	8.33E−01	7.76E−01	1.61E+00	1.17E+01
	HTP, kg DCB-eq	5.72E+00	1.04E+00	5.72E−01	1.62E+00	5.93E+00
Sodium hypochlorite (13 % w/w)	GWP, kg CO <sub>2</sub> -eq	3.58E+02	1.45E+02	1.96E+02	3.41E+02	4.09E+02
	PE, GJ	4.05E+00	1.60E+00	1.32E+00	2.92E+00	4.12E+00
	WU, ML	4.70E−02	5.15E−04	4.55E−04	9.71E−04	4.71E−02
	FETP, kg DCB-eq	1.46E−01	3.90E−03	3.44E−03	7.34E−03	1.47E−01
	METP, kg DCB-eq	1.10E+04	2.77E+02	2.14E+02	4.92E+02	1.10E+04
	TEP, kg DCB-eq	4.31E+00	4.40E−01	2.12E−01	6.52E−01	4.34E+00
	HTP kg DCB-eq	2.84E+00	5.51E−01	1.92E−01	7.43E−01	2.88E+00
Ferric chloride (42 % w/w)	GWP, kg CO <sub>2</sub> -eq	1.16E+03	2.63E+02	6.87E+02	9.50E+02	1.33E+03
	PE, GJ	1.24E+01	2.92E+00	3.49E+00	6.40E+00	1.27E+01
	WU, ML	6.68E−02	9.37E−04	1.34E−03	2.28E−03	6.71E−02
	FETP, kg DCB-eq	2.82E−01	7.09E−03	2.50E−02	3.20E−02	2.85E−01
	METP, kg DCB-eq	1.61E+04	5.04E+02	1.79E+03	2.30E+03	1.63E+04
	TEP, kg DCB-eq	1.13E+01	8.01E−01	9.35E−01	1.74E+00	1.14E+01
	HTP, kg DCB-eq	4.71E+00	1.00E+00	1.29E+00	2.30E+00	4.85E+00
Aluminium sulphate (47 % w/w)	GWP, kg CO <sub>2</sub> -eq	2.38E+02	3.00E+02	3.25E+02	6.24E+02	3.87E+02
	PE, GJ	4.86E+00	3.32E+00	1.66E+00	4.98E+00	5.04E+00
	WU, ML	5.59E−02	1.07E−03	9.91E−04	2.06E−03	5.62E−02
	FETP, kg DCB-eq	6.54E−01	8.07E−03	1.92E−01	2.00E−01	6.56E−01
	METP, kg DCB-eq	3.64E+04	5.74E+02	1.20E+04	1.26E+04	3.65E+04
	TEP, kg DCB-eq	5.33E+00	9.12E−01	4.33E+00	5.24E+00	5.41E+00
	HTP kg DCB-eq	3.89E+00	1.14E+00	1.30E+01	1.42E+01	4.00E+00
Fluorosilicic acid (22 % w/w)	GWP, kg CO <sub>2</sub> -eq	1.82E+02	3.51E+02	1.12E+03	1.47E+03	5.69E+02
	PE, GJ	5.16E+00	3.89E+00	4.60E+00	8.49E+00	5.60E+00
	WU, ML	9.97E−02	1.25E−03	3.35E−03	4.60E−03	1.00E−01
	FETP, kg DCB-eq	1.39E−01	9.46E−03	1.91E−01	2.00E−01	1.45E−01
	METP, kg DCB-eq	4.89E+03	6.72E+02	1.20E+04	1.26E+04	5.23E+03
	TEP, kg DCB-eq	3.47E+00	1.07E+00	4.44E+00	5.51E+00	3.66E+00
	HTP, kg DCB-eq	1.23E+00	1.34E+00	1.15E+01	1.29E+01	1.51E+00
Calcium oxide	GWP, kg CO <sub>2</sub> -eq	1.31E+03	1.59E+02	3.87E+02	5.47E+02	1.37E+03
	PE, GJ	8.13E+00	6.58E−01	1.26E+00	1.92E+00	8.20E+00
	WU, ML	1.91E−02	2.20E−05	4.04E−04	4.26E−04	1.92E−02
	FETP, kg DCB-eq	4.87E−02	4.27E−03	5.29E−03	9.56E−03	4.96E−02
	METP, kg DCB-eq	2.53E+03	3.81E+02	3.28E+02	7.09E+02	2.58E+03
	TEP, kg DCB-eq	1.93E+00	5.61E−01	2.34E−01	7.95E−01	1.97E+00
	HTP, kg DCB-eq	8.61E−01	1.17E−01	1.69E−01	2.85E−01	9.03E−01
Chlorine gas	GWP, kg CO <sub>2</sub> -eq	1.72E+03	1.18E+03	9.19E+02	2.10E+03	1.89E+03
	PE, GJ	1.92E+01	1.31E+01	6.39E+00	1.95E+01	1.95E+01
	WU, ML	2.41E−01	4.20E−03	1.24E−03	5.44E−03	2.41E−01
	FETP, kg DCB-eq	7.29E−01	3.18E−02	2.41E−02	5.58E−02	7.32E−01
	METP, kg DCB-eq	5.02E+04	2.26E+03	1.51E+03	3.76E+03	5.04E+04
	TEP, kg DCB-eq	1.40E+01	3.59E+00	1.18E+00	4.76E+00	1.41E+01
	HTP, kg DCB-eq	1.29E+01	4.49E+00	1.44E+00	5.93E+00	1.31E+01

generators' accounts but as a one-off fee permit issued by the relevant State Government (NWC 2009). This can be confirmed when the water use figures from the ABS (2012) for the electricity generation sector of Australia shows only 327,834 ML in the category "consumption" but 44,483,500 ML in the category "in-stream use". The importance of using hybrid modelling is shown again by taking advantage of the detailed data regarding water use for electricity generation, including river water and lake water, from the GaBi 5 database (PE International 2012).

Freshwater and marine ecotoxicity results using IO modelling were smaller than equivalent process-based results for all of the chemicals under study except fluorosilicic acid. Further inspection of the IOA results for this chemical indicated that the zero order constitutes less than 5 % of the final result for both indicators and process-based results indicate that most impacts are located upstream, associated with selenium and antimony emissions from sulphuric acid production. Additionally, a possible factor to be considered in the differences between the zero and higher order results in IOA is the high price of tradable commodities such as sulphuric acid, phosphate rock and bauxite in 2008 (WRF 2009). This impact can also be identified in the higher order results for aluminium sulphate which uses sulphuric acid as raw material. The impact on the expenditure vector from the change in tradable commodity prices is further explained in Section 3.3 and seems less relevant for chlor-alkali chemicals.

In the case of terrestrial ecotoxicity and human toxicity potentials, IOA results are generally lower than process-based results with the exception of aluminium sulphate and fluorosilicic acid. Inspecting the IOA results, we found that most of the impacts for chlor-alkali chemicals are at the zero-order level, while for aluminium sulphate and fluorosilicic acid, the higher orders have the biggest contribution (>80 %). In particular, substantial burden is produced by the

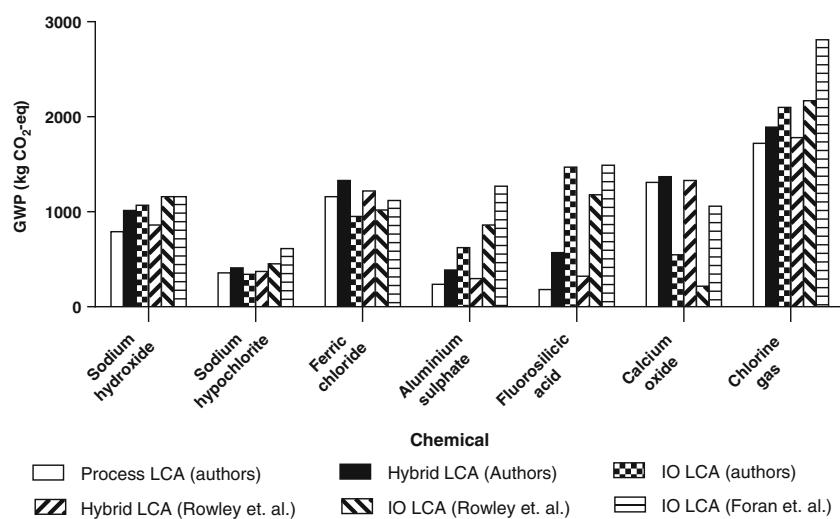
"Basic non-ferrous metal manufacturing" sector, which provides raw materials (sulphuric acid and alumina) and is the biggest contributor to HTP and the second biggest to TETP results in Australia. The main reasons for the large higher order results for HTP and TETP are arsenic and sulphur dioxide emissions to air from ore processing of non-ferrous metals.

### 3.2 Comparison with previous studies

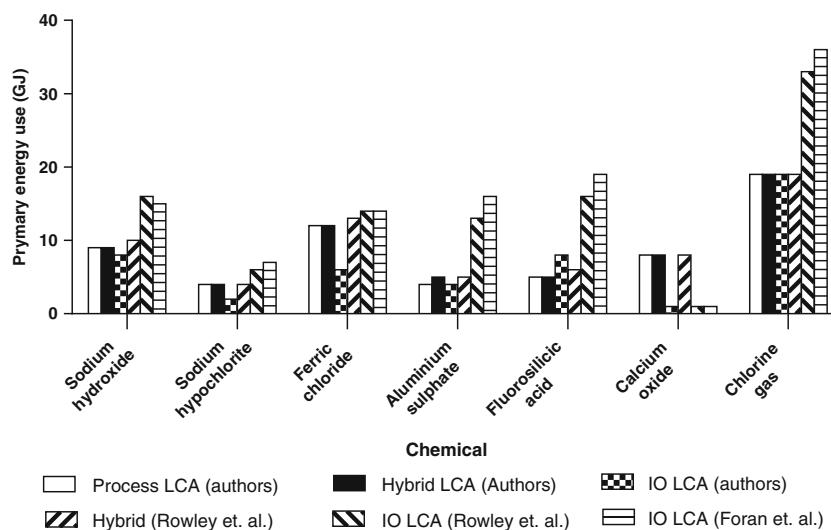
We have compared our results with those of two prior IOA and hybrid studies (Rowley et al. 2009; Foran et al. 2005) which used Australian input–output tables for 1998–1999 and 1994–1995, respectively, and deflated the unit prices of chemicals and expenditures used in our model to 1998–1999 and 1994–1995 prices using producer price index data at the class and subdivision level (ABS 2011c). A graphical comparison between studies is shown in Figs. 2, 3 and 4 for GWP, PE and WU, respectively. Comparisons of results for the various ecotoxicity and human toxicity impact assessment categories are not presented due to differences between hybrid models.

In general, GWP results were within the same order of magnitude using any of the three IO models (see Fig. 2), with larger gaps between them for calcium oxide and aluminium sulphate. For calcium oxide, most of the GWP impact is associated with the zero level, which, as shown in Fig. 2, is better simulated using process modelling than IOA. In contrast, aluminium sulphate, which is included in the basic chemical sector, has little GWP impact at the zero level but has a much more important GWP impact upstream of the supply chain due to bauxite processing and the co-production of sulphuric acid in non-ferrous metal production. For this chemical, process modelling tended to underestimate the impacts while IOA allowed us to capture better the upstream impacts described

**Fig. 2** GWP for water treatment chemicals using process, hybrid and input–output modelling



**Fig. 3** PE for water treatment chemicals using process, hybrid and input–output modelling



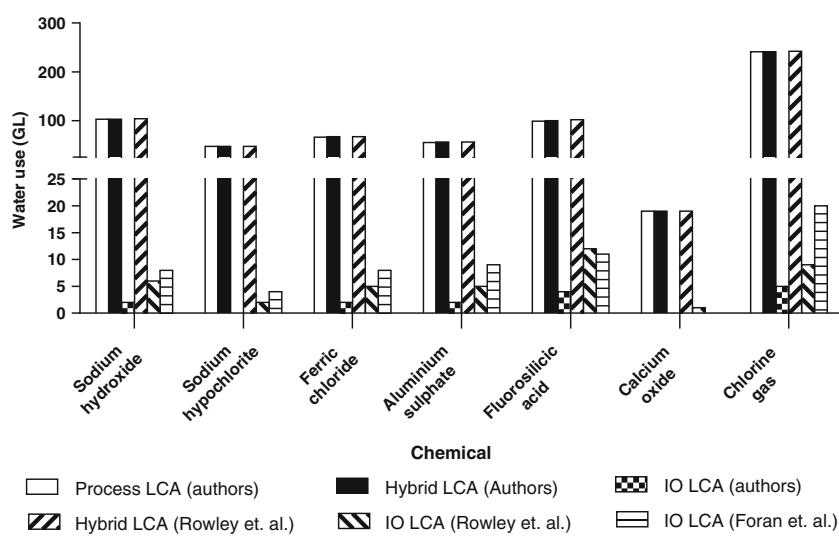
above. In all cases, hybrid modelling was able to compensate for the weaknesses of both individual approaches and provide a more meaningful answer.

Regarding primary energy use, the results of Rowley et al. (2009) and Foran et al. (2005) for all chemicals (except calcium oxide which belong to the IOIG Cement, lime and ready-mixed concrete) were consistently higher than both the process-based results and the IO results of the current study (see Fig. 3). Inspection of the underlying IOA data revealed differences in the primary energy values for the Basic chemicals sector between the three models. Direct contributions were 7.9 MJ/AUD (authors) versus 24.4 MJ/AUD (Rowley et al. 2009) and 27.4 MJ/AUD (Foran et al. 2005). Total contributions were 18.4 MJ/AUD (authors) versus 41.5 MJ/AUD (Rowley et al. 2009) and 39.0 MJ/AUD (Foran et al. 2005). Primary energy use by the Basic chemical sector has been relatively flat while the output of this sector has increased, in nominal terms, from AUD 5,974 million to AUD 17,418 million, yielding a much lower megajoule/AUD

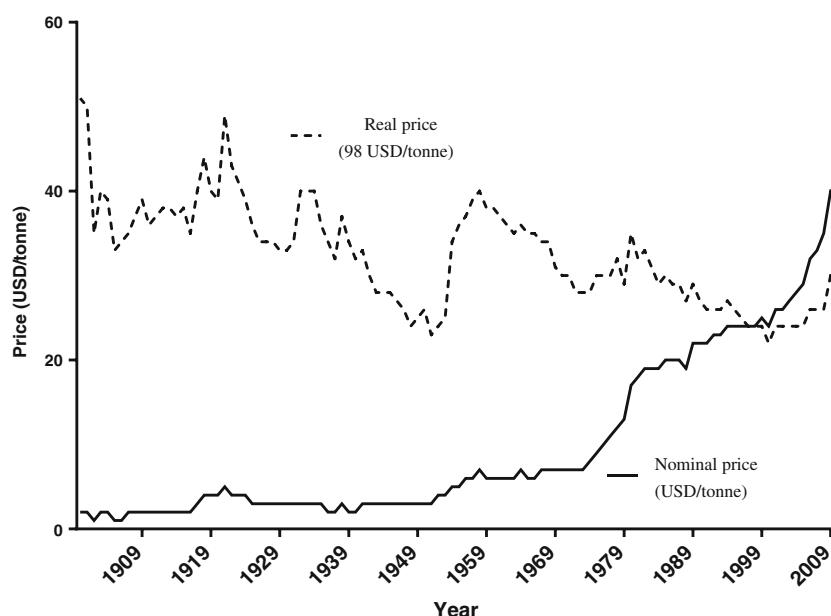
ratio for the authors' model. Although the price of chemicals was deflated to the other models' reference years for comparison, the deflation does not account for real price increases over time.

Regarding water use, the process-based results appear overestimated when compared with any of the IOA results (see Fig. 4); however, in the case of sodium hydroxide, sodium hypochlorite, chlorine gas and ferric chloride, more than 75 % of the water use in the process-based model is associated with the supply of electricity to the membrane cells used in production. In the case of aluminium sulphate and fluorosilicic acid, the water is mainly used in the production of sulphuric acid. In the case of calcium oxide, the water is mainly used in washing limestone. Identifying these contributing factors helps explain the trend observed and again reinforces the value of hybrid modelling, as these impact contributions were largely unaccounted for by the IOA model alone due to that model's averaging of results across the sector.

**Fig. 4** Water use for water treatment chemicals using process, hybrid and input–output modelling



**Fig. 5** Nominal and real prices of commodity salt during the last 100 years (USGS 2011). Nominal prices are shown for salt in original dollar terms and real prices are expressed in 1998 USD equivalent figures after inflation has been taken into account



### 3.3 Sensitivity of results to the assumed wholesale prices

Input–output tables are often published by statistical bureaux with a lag time of up to 5 years, while prices used to estimate zero and higher order burdens in IOA change continuously. While it is commonly accepted that technical coefficients in IO tables are stable for mature technologies such as those used for the production of basic chemicals, the raw materials used in their production processes (e.g. salt) might be subject to significant price volatility as shown in Fig. 5.

Variability in prices is especially relevant for aluminium sulphate and fluorosilicic acid, which are linked to commodities such as sulphuric acid, phosphate rock and bauxite. To compare the sensitivity of the hybrid results to the assumed wholesale prices, these have been deflated to Australian dollars in the reference year of the IO table being used in this study (2007–2008). The impacts of price volatility on the absolute results of the hybrid modelling for GWP are shown in Table 2. The last two columns of the table show the reduction of the

variability in the results, measured using the coefficient of variation (CoV), before and after the hybridisation using the pure IO modelling as the base case. As shown in Table 2, price fluctuations in raw materials can lead to variation in the hybrid results as small as 1 % for calcium oxide and as big as 59 % for fluorosilicic acid, with chlor-alkali chemicals showing differences lower than 5 %. The hybrid model shows less sensitivity to commodity prices than the pure IO model, which can vary up to 149 % for fluorosilicic acid.

The depth of the interface between the process and IO model also has a vital role in the robustness of the hybrid results to commodity price variability. Most supply chains described in this study are covered by the process model up to the fourth level of depth, and we expect that the higher order contributions of the IOA to the final results in the hybrid model are smaller than those from the process-based analysis. If the process model was shallower, then we might expect the hybrid results to be more sensitive to price fluctuations.

**Table 2** Variability of GWP results in the hybrid model presented here due to changes in raw material prices (2005–2010)

Chemical	GWP (kg CO <sub>2</sub> -eq) per tonne						Variability	
	2005	2006	2007	2008	2009	2010	CoV <sub>IOA</sub>	CoV <sub>Hybrid</sub>
Sodium hydroxide	1.079	1,092	1,023	1,014	995	1,003	0.21	0.04
Sodium hypochlorite	415	427	410	409	405	406	0.22	0.02
Ferric chloride	1,289	1,298	1,313	1,328	1,290	1,316	0.13	0.01
Aluminium sulphate	335	350	342	387	330	323	0.27	0.07
Fluorosilicic acid	264	266	287	569	271	343	0.76	0.36
Calcium oxide	1,371	1,373	1,369	1,367	1,355	1,349	0.22	0.01
Chlorine gas	1,886	1,924	1,864	1,890	1,852	1,853	0.26	0.01

#### 4 Conclusions and recommendations

The authors have developed a hybrid database for water treatment chemicals and have compared the results of hybrid LCA with those of equivalent process- and IO-based analyses. The hybridisation has demonstrated not only the advantages of expanding the system boundaries in the modelling but also the importance of using detailed information at the process level. Moreover, where there are important price fluctuations in the raw materials used for the production of these industrial commodities, hybrid modelling provided a more robust output.

This study has also enabled the evaluation of LCA results from different attributional perspectives, for example, GWP results for chlor-alkali chemicals using IOA were closer to the process-based results than was expected, while hybrid modelling provided a more meaningful outcome for aluminium sulphate, fluorosilicic acid and calcium oxide for this impact category.

Detailed environmental interventions data remain a challenge to gather in Australia. The progressive release of environmental accounts by the ABS following recommendations from the United Nations will enable more widespread future use of IO modelling which is fundamental in the construction of hybrid models. A free Australian online input–output tool, like EIO-LCA (Carnegie Mellon University Green Design Institute 2012), would be helpful in the future development of hybrid models for other Australian industry sectors.

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